

Absence of topological degeneracy in the Hubbard model on honeycomb lattice

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It is shown that the unique sign structure of the ground state of the Hubbard model on honeycomb lattice, which is shown to be insensitive to the trapped Z_2 gauge flux when the system is defined on a torus, may cause the absence of topological degeneracy on this bipartite system. Examples of variational Mott insulating state on the honeycomb lattice are given to illustrate the close relation between the sign structure of the ground state and the (absence of) topological degeneracy.

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The search for spin liquid ground state is a central issue in the study of the strongly correlated electron systems. The spin liquid state represents a novel state of matter beyond the Landau-Ginzburg description and supports new kinds of order and excitation. It is generally believed that the study of spin liquid state will not only deepen our understanding on the organizing principles of condensed matter systems, but also result in new applications that is not possible from conventional materials. In particular, the topological order and the related fractionalized excitations are proposed to implement the key steps of topological quantum computation.

It is generally believed that the geometrically frustrated quantum antiferromagnetic systems are ideal places to find spin liquid ground state. For this reason, the study of Heisenberg model on Kagome lattice and triangular lattice have received considerable interests. More recently, the spin liquid states are also proposed to appear in Hubbard models on frustrated lattices as a result of the multi-spin exchange processes. The bipartite lattice, on which the antiferromagnetic exchange interaction is not frustrated, is generally not believed to be favorable for the formation of the spin liquid ground state. For example, on the square lattice, the system develops magnetic long range order as soon as one turns on the electron correlation. With these understandings in mind, it is quite unexpected that a spin liquid ground state can exist in the Hubbard model on the bipartite honeycomb lattice.

According to the numerical results reported recently by Meng et. al[1], a state with full gaps to both charge and spin excitations and full symmetry of the Hamiltonian emerges in a small interaction range of $3.5 < U/t < 4.2$ for the Hubbard model on honeycomb lattice. This state intervenes between a semimetal phase with a Dirac-type spectrum for $U/t < 3.5$ and an antiferromagnetic ordered phase with spin wave excitation for $U/t > 4.2$, resulting in a counterintuitive non-monotonic evolution of the spin excitation spectrum with U/t . What makes this state even more special is that although it has a full gap to spin excitation, it has no accompanying topological degeneracy.

In a loose sense, a spin liquid state can be defined as

a quantum disordered insulating state of a many electron system that respect all the symmetries of the Hamiltonian. However, to exclude the trivial case of a band insulator, in which the spin degree of freedoms cancel out in each unit cell, one should add the further requirement that each unit cell of the lattice contains an odd number of electrons. A system with an odd number of electrons in each unit cell will inevitably possess gapless excitations at the mean field level if there is no symmetry breaking mechanism to enlarge the unit cell[3]. Built on the higher dimensional generalization of the celebrated Lieb-Schultz-Mattis theorem in one dimension, it is now generally believed that a spin liquid state should either be gapless, or, while possessing a bulk gap to spin excitation, show topological degeneracy[2]. The topological degeneracy denotes the degeneracy between ground states that can not be distinguished locally but are globally distinct. The existence of topological degeneracy is one of the most important manifestation of topological order, which is believed to be a prerequisite for the emergence of fractionalized excitations in the spin liquid background[4]. For these reasons, it is not surprising that the negative result on the topological degeneracy reported by Meng et.al. in the spin liquid state has aroused much interests and also confusions in the community[5–8].

In a sense, the absence of topological degeneracy in the Hubbard model on honeycomb lattice should not be that surprising since the honeycomb lattice is a complex lattice with two inequivalent sites in each unit cell. A state with one electron per site on average actually corresponds to integer filling rather than half filling. Thus the above mentioned hypothesis on the topological degeneracy should not apply here. However, it is not clear to what extent is the oddness of electron number in each unit cell essential for the existence of the topological degeneracy in a fully gaped system. As the topological degeneracy is the key to the exoticness of a spin liquid[4] and as some doubts have been raised on the negative results of topological degeneracy[7, 8] in the numerical work, it is valuable to understand if Hubbard model on honeycomb can really support topological degeneracy. Even leaving apart the topological degeneracy, it is still a challenging task to compose a picture for the spin liquid

state reported in the numerical works and to understand how a full gap can be generated in the spin excitation spectrum without breaking any symmetry[5–8].

In this paper, we provide an analytical argument for the absence of topological degeneracy in the Hubbard model on honeycomb lattice. This argument is based on the unique sign structure of the ground state of this bipartite system, which is shown to be insensitive to the trapped gauge flux when the system is defined on a torus. To illustrate the effect of the ground state sign structure on the topological degeneracy, we also present the results of a variational study on some Mott insulating states on the honeycomb lattice.

The model studied in this paper reads

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

in which the first sum is over nearest neighboring sites on the honeycomb lattice. The honeycomb lattice is a complex lattice with two inequivalent sites in each unit cell (see Fig.1) and can be divided into two sublattices (even and odd). The hopping terms are nonzero only between sites on different sublattices. With \vec{b}_1 and \vec{b}_2 denoting the primitive lattice vectors in reciprocal space ($\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{i,j}$), the momentum in the Brillouin zone can be parameterized as $\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2$. The kinetic part of the Hamiltonian can then be diagonalized as follows

$$H_0 = \sum_{k\sigma,s} E_{k,s} \gamma_{k\sigma,s}^\dagger \gamma_{k\sigma,s}, \quad (2)$$

in which $E_{k,s} = s|1 + e^{ik_1} + e^{ik_2}|$ and $s = \pm 1$. $\gamma_{k\sigma,s}$ is corresponding eigen-operator. The bare dispersion has two Dirac points at $(k_1, k_2) = \pm(2\pi/3, -2\pi/3)$ in the first Brillouin zone. When the electron density is such that there is one electron per site on average, the Fermi surface of the free system shrinks into these two Dirac points. Thus, although the honeycomb lattice is bipartite and the antiferromagnetic interaction is not frustrated, a finite strength of local correlation is needed to induced the instability of spin density wave ordering.

It should be noted that the gaplessness of the bare dispersion at $(k_1, k_2) = \pm(2\pi/3, -2\pi/3)$ is protected by the bipartite nature and the three-fold rotational symmetry of the honeycomb lattice. Supposing that the hopping integral is nonzero only between sites on different sublattices, then by the three-fold rotational symmetry, a hopping term between sites separated by an arbitrary vector $\vec{R}_1 = (m + \frac{1}{3})\vec{a}_1 + (n + \frac{1}{3})\vec{a}_2$ is always accompanied by two other hoppings of the same amplitudes at separations $\vec{R}_2 = -(m + n + \frac{2}{3})\vec{a}_1 + (m + \frac{1}{3})\vec{a}_2$ and $\vec{R}_3 = (n + \frac{1}{3})\vec{a}_1 - (m + n + \frac{2}{3})\vec{a}_2$. It is then easy to check that the expression $\sum_{i=1,2,3} e^{i\vec{k} \cdot \vec{R}_i}$ is identically zero at $(k_1, k_2) = \pm(2\pi/3, -2\pi/3)$. The same argu-

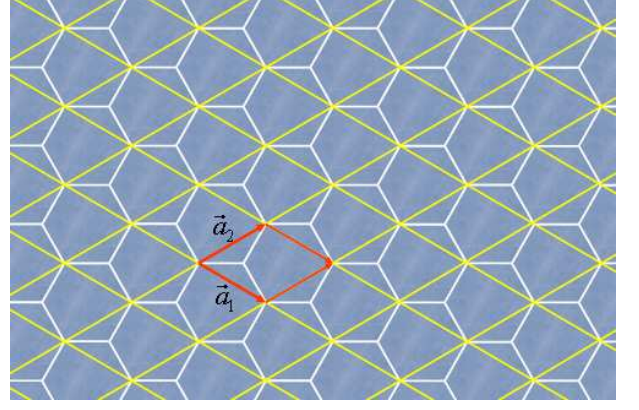


FIG. 1: The honeycomb lattice and its unit cell.

ments can also be used to show that BCS pairing between sites on the different sublattices and respecting the three-fold rotational symmetry can neither open a gap at $(k_1, k_2) = \pm(2\pi/3, -2\pi/3)$.

With this in mind, it is then quite unusual that a full gap in both spin and charge sector can be opened without any symmetry breaking. Could it be possible that the system spontaneously violates the bipartite nature of the honeycomb lattice by generating hopping or pairing terms between sites on the same sublattice[7, 8]? The analytical argument present below suggests that this is very unlikely to be the case. The same argument also provides an understanding on the absence of the topological degeneracy in the Hubbard model on honeycomb, or more generally, bipartite lattice.

Our argument is based on the now well known Lieb's theorem on the sign structure of the ground state on bipartite lattice for the Hubbard model. On a bipartite lattice such as the honeycomb lattice studied in this paper, the Hubbard model is particle-hole symmetric. To be more specific, through the following unitary transformation

$$\begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix} \longrightarrow \begin{pmatrix} c_{i\uparrow} \\ \eta_i c_{i\downarrow}^\dagger \end{pmatrix}, \quad (3)$$

in which $\eta_i = -1$ for i in the odd sublattice and is otherwise 1, the Hubbard model takes the form

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) - U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (4)$$

up to a chemical potential term. Under such a transformation, a repulsive Hubbard model is mapped into an attractive Hubbard model. At the same time, the spin and charge degree of freedoms interchange their roles in the particle-hole transformed system. For example, a repulsive system with one electron per site is mapped into an attractive system with zero magnetization.

In a celebrated paper appeared in 1989 by Lieb[10], it is proved that the attractive Hubbard model Eq.(4) on

any lattice has a unique ground state with a well defined sign structure. More specifically, if we use the Fock basis $|\alpha, \uparrow\rangle = \prod_k c_{i_{\alpha k} \uparrow}^\dagger |0\rangle$ and $|\alpha, \downarrow\rangle = \prod_k c_{i_{\alpha k} \downarrow}^\dagger |0\rangle$ to expand the ground state as $|\Psi\rangle = \sum_{\alpha, \beta} \phi_{\alpha, \beta} |\alpha, \uparrow\rangle \otimes |\beta, \downarrow\rangle$, then the coefficient matrix ϕ (whose matrix elements are amplitudes of the ground state in the Fock basis) can be shown to be positive definite, although in general its matrix elements can be negative as a result of the Fermion sign. This can be understood as a result of the local attractive interaction which encourages the down spin electrons to follow the trail of the up spin electrons. In particular, the ground state amplitude is positive definite when electrons of both spins share the same set of lattice sites. In term of the repulsive Hubbard model before the particle-hole transformation, this corresponds to a singly occupied configuration. Keep in mind the alternative sign η_i in the particle-hole transformation Eq.(3), it can be shown easily that in the repulsive Hubbard model, the ground state amplitudes in the singly occupied subspace satisfy the so called Marshall sign rule. The Marshall sign rule claims that the ground state amplitudes in the singly occupied subspace are real and their signs are given by $(-1)^{N_{\downarrow}^{even}}$ up to a global phase factor. Here N_{\downarrow}^{even} is the number of down spin electrons in the even sublattice.

The existence of such a sign structure in the ground state, which is a result of bipartite nature of the honeycomb lattice, makes it very unlikely that the reported spin gap is generated by intra-sublattice hopping or pairing terms[7, 8]. At the same time, the sign structure of the ground state provides a way to understand the absence of the topological degeneracy in this system. To appreciate this point, it is crucial to realize that Lieb's proof is general enough to address not only the sign structure of the ground state, but also its response to the trapped gauge flux when the system is defined on a torus. Lieb's proof applies whenever the lattice is bipartite, while up to a gauge transformation trapping a gauge flux in the holes of the torus amounts simply to change the phase of the hopping integrals on the bonds across the boundary of the system. Thus, the ground state after the gauge flux trapping has exactly the sign structure as that before the gauge flux trapping up to an inessential global phase. It is just this boundary condition independence of the sign structure of the ground state that enables us to arrive at our conclusion.

To be more specific, the discussion below will be restricted to the topological degeneracy of the Z_2 type, which is the most commonly envisaged in a gapped quantum spin liquid[9]. A scheme to detect topological degeneracy in the resonating valence bond (RVB) state generated from Gutzwiller projection of BCS mean field state is proposed by Ivanov and Senthil in 2002[12]. They proposed to check the orthogonality between RVB states with different number of trapped visons (the Z_2 topological excitation) in the holes of a multiply connected

manifold. For a topological ordered system, states with different number of trapped visons in the holes are orthogonal to each other and form topological degeneracy. On the other hand, for a topological trivial state, the visons can tunnel through the bulk of the system and escape from the holes. The topological degeneracy is lifted by such tunneling events. Built on the conceptual link in the RVB picture between a quantum spin liquid and a quantum phase disordered superconductor, Ivanov and Senthil also proposed to construct the vison excitation from quantized superconducting vortex in the mean field state. It is then found that as a result of the Z_2 character of the quantized superconducting vortex, trapping a vison in a hole of multiply connected manifold for the RVB state amounts to changing the boundary condition around the hole from periodic to anti-periodic or vice versa.

In a later generalization by the present author and Yang[13], the role of the superconducting vortex in defining the vison is replaced by that of a Z_2 gauge flux. Thus, to detect topological degeneracy in the RVB state, one should check the sensitivity of the ground state to a quantized gauge flux in the holes on a multiply connected manifold. Such a definition closely resembles the way that Kohn chose to define an insulator[11]. According to this definition, the key difference between an insulator showing topological degeneracy (order) and a trivial insulator is that the former can respond nonlocally to a trapped Z_2 gauge flux while the latter has no such non-local response.

In [13], it is also shown that RVB states generated from bipartite mean field Hamiltonian through Gutzwiller projection all satisfy the Marshall sign rule, no matter what is the gauge structure of the corresponding effective theories at the Gaussian level. As a result of such sign structure, it is proved generally that all RVB state generated from a bipartite mean field Hamiltonian can not support topological order. The same argument can also be adopted here after some modifications. The modification is necessary for two reasons. First, here we are discussing ground state of a given Hamiltonian rather than a general RVB state with unspecified Hamiltonian. Second, the model we discuss here also has charge excitation, the existence of which will inevitably cause Fermion sign and the ground state wave function has a definite sign only in the subspace of singly occupied state.

To deal with the first problem, we simply introduce the Z_2 gauge flux directly in the Hamiltonian rather than in the effective theory as was done in the previous study. From the above argument on the topological degeneracy, this seems to be intuitively even more appealing as it allow us to probe directly the response of the ground state to the trapped Z_2 gauge flux.

Now we check the orthogonality of the ground states with and without a trapped Z_2 gauge flux in the holes of a multiply connected manifold. Let ϕ and ϕ' be the wave

function matrixes of the ground states $|\Psi\rangle$ and $|\Psi'\rangle$ before and after the flux trapping, then as the sign structure of the ground state is insensitive to the trapped gauge flux, both matrixes should be positive definite up to a global phase factor. The overlap of the two states is given by $\langle\Psi|\Psi'\rangle = \text{Tr}\phi\phi'$, in which we have used the fact that both ϕ and ϕ' can be assumed to be Hermitian without loss of generality. In the diagonal representation of ϕ , the overlap can be written as $\langle\Psi|\Psi'\rangle = \sum_i w_i \phi'_{i,i}$, in which w_i are the positive definite eigenvalues of the matrix ϕ and $\phi'_{i,i}$ are the diagonal matrix elements of matrix ϕ' in this representation. Since ϕ' is also positive definite, $\phi'_{i,i} > 0$. Thus the overlap is the sum of positive terms and is nonzero for finite system.

To prove the absence of the topological degeneracy, one should still go to the thermodynamic limit to see if the overlap converges to a finite value. At present a proof of this is beyond our reach. With this in mind, the results presented above can be either interpreted as a suggestive evidence for the absence of the topological degeneracy, or, on the other way around, an excuse for the failure to detect the anticipated topological degeneracy on finite system. However, forbiddenness of topological degeneracy induced by the Marshall-sign structure of ground state has been illustrated before at the variational level for various RVB states and the same thing can also be done for the honeycomb system.

For this purpose, we investigate two typical Mott insulating states on the honeycomb lattice with built-in Marshall sign structure. Both of these states are generated by Gutzwiller projection of BCS mean field states. The first is the Gutzwiller projection of the free Fermion state on the honeycomb lattice with nearest neighboring hopping terms and two Dirac points at $(k_1, k_2) = \pm(2\pi/3, -2\pi/3)$. The second is the Gutzwiller projection of the BCS pairing state with $d+id'$ pairing pattern between neighboring sites[14]. The Z_2 gauge flux can be imposed in the boundary condition of the BCS mean field Hamiltonian[12, 13].

As a result of a general theorem proved in [13], both states satisfy the Marshall sign rule, even if the unprojected wave function is not real(as for the $d+id'$ state). To see if topological degeneracy can survive in these states, we calculate the overlap of the states defined on a torus with different number of Z_2 gauge flux threaded in both holes of the torus. The overlap between the wave functions can be easily calculated by with the variational Monte Carlo method. The results for the projected free Fermion state is presented in Fig. 2, in which we have shown the overlap between the state with no flux in both holes and the state with Z_2 flux in one hole and no flux in the other hole of the torus. The calculation is done on lattice with $L \times L \times 2$ sites and L is so chosen to avoid the Dirac nodes in the momentum space. The results rapidly converges to a finite value when $L > 10$.

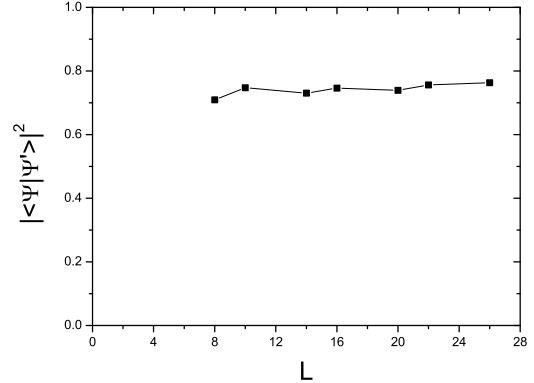


FIG. 2: The overlap between states with different number of Z_2 gauge flux in both holes of the torus for the Gutzwiller projected free Fermion state on honeycomb lattice. $|\Psi\rangle$ denotes the state with no gauge flux in both holes of the torus and $|\Psi'\rangle$ denotes the state with Z_2 gauge flux in one hole but no flux in the other hole of the torus.

An even more striking example of how the sign structure of the ground state can cause the absence of the topological degeneracy is provided by the projected $d+id'$ wave pairing state on the honeycomb lattice. Here, the unprojected mean field state break the time reversal symmetry and has a complex wave function. In terms of the effective field theories[9], the RVB state generated from such a mean field ansatz would possess a Z_2 gauge structure and thus support topological order. However, after the Gutzwiller projection, the wave function becomes real up to a global phase and satisfies the Marshall sign rule. In Fig.3 we present the overlap of the state with Z_2 gauge flux in the hole surrounded by the x-circumference but no flux in the hole surrounded by the y-circumference (denoted as $|\Psi_{10}\rangle$) and the state with Z_2 gauge flux in the hole surrounded by the y-circumference but no flux in the hole surrounded by the x-circumference (denoted as $|\Psi_{01}\rangle$). The overlap is also seen to converge to a finite value in the thermodynamic limit.

Although both variational states presented above are not meant to describe the spin liquid state found in the numerical simulation of [1], they do illustrate well how the sign structure of the ground state can cause the non-orthogonality of the states with and without trapped gauge flux in the thermodynamic limit and thus the forbiddenness of the topological degeneracy of the system. A full description of the spin liquid state found in [1] is beyond the scope of this paper and requires obviously further refinement of the variational wave function. For example, the virtual charge fluctuation should obviously be taken into account. However, we think these modifications will not change our conclusion qualitatively.

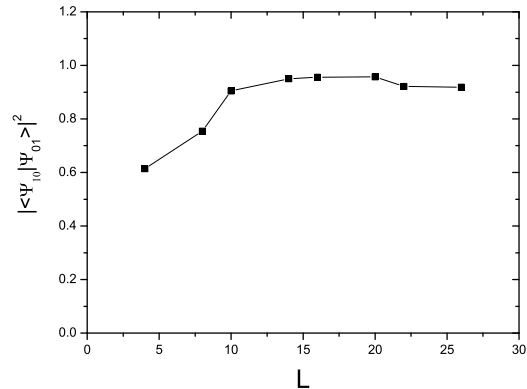


FIG. 3: The overlap between states with different number of Z_2 gauge flux in both holes of the torus for the Gutzwiller projected $d + id'$ pairing state on honeycomb lattice. $|\Psi_{10}\rangle$ denotes the state Z_2 gauge flux in the hole surround by the x-circumference but no flux in the hole surrounded by the y-circumference and $|\Psi_{01}\rangle$ denotes the state with Z_2 gauge flux in the hole surround by the y-circumference but no flux in the hole surrounded by the x-circumference.

In summary, we have presented both analytical arguments and variational examples that suggest the topological degeneracy can not survive in the Hubbard model on honeycomb lattice as a result of the unique sign structure of its ground state. The same sign structure is believed to be important also for other aspects of the ground state and should be taken into account in the variational study.

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